5. Majoranas in topological superconductors-a

Particle-hole symmetry

In recent years, the idea of a Majorana fermion was resurrected in the context of condensed matter where it could be realized as a quasiparticle in a superconductor. Intuitively it is natural to search in a superconductor because quasiparticle excitations contain both particle and hole degrees of freedom. A hole is simply the "antiparticle" of an electron.

In the language of creation and annihilation operators, the charge conjugation operation discussed previously is simply the operation of taking the Hermitian conjugate. At mean field level, the Hamiltonian for a superconductor in the second quantification reads

$$H = \frac{1}{2}\mathcal{C}^\dagger \mathcal{H} \mathcal{C}$$

with $\mathcal{C}^\dagger = (c^\dagger, c)$ and c is a row/column vector comprising the annihilation operators at all the lattice sites in a superconductor, eventually with a spin index ($c_\uparrow$ or $c_\downarrow$). The Bogoliubov-de Gennes Hamiltonian reads

$$\mathcal{H}_{BdG} = \begin{pmatrix} \mathcal{H}_0 & \Delta \\ \Delta^\dagger & -\mathcal{H}_0^* \end{pmatrix}$$

where Δ is the matrix containing the superconducting order parameters. The action of the charge conjugation transformation is to convert a particle into a hole and vice versa

$$\mathfrak{C} c \mathfrak{C}^{-1} = c^\dagger$$

The Hamiltonian exhibits the charge conjugation symmetry

$$[\mathfrak{C}, H] = 0$$

Together with the Hermiticity of $\mathcal{H}_{BdG}$, it is sufficient to determine the consequences of charge conjugation symmetry on the BdG Hamiltonian,

$$\mathfrak{C}\mathcal{H}_{BdG}\mathfrak{C}^{-1} = \tau_1 \mathcal{H}_{BdG} \tau_1 = -\mathcal{H}_{BdG}^*$$

where τ are the usual Pauli matrices acting in particle-hole space. This allows to define a particle-hole symmetry represented by an anti-unitary operator $\mathfrak{C}'$ that anticommutes with the Hamiltonian. Note that it is not a proper symmetry, due to the anticommutation

$$[\mathfrak{C}', \mathcal{H}_{BdG}] = 0 \quad \text{with} \quad \mathfrak{C}' = \tau_1 K$$

and K the complex conjugation operator. The consequence of this property is that any eigenstate of the BdG Hamiltonian has a particle-hole conjugate with opposite energy. That is, the presence of the PHS immediately reflects itself as redundancy in the solutions to the BdG equations. For example, take the Schrödinger equation

$$\mathcal{H}_{BdG}\Psi = E\Psi, \quad \Psi^T = (u^T, v^T)$$

where u/v stands for the particle/hole component of the wave function. The solutions describe the quasiparticles excitations above the BCS ground state. Then if (u^T, v^T) is the solution with energy E, then $(v^\dagger, u^\dagger)$ is the particle-hole conjugate with energy $-E$. In contrast, a quasiparticle solution is a Majorana fermion if it is equal to its own particle-hole conjugate (anti-quasiparticle), at the same energy. This implies that a Majorana fermion can be realized only at zero energy.

A solution to the mean-field equation can also be represented by a quasiparticle creation operator

$$\gamma_E^\dagger = \sum_j u_{j,E} c_j^\dagger + v_{j,E} c_j$$

where j runs over all the sites (orbitals, and spins) in the superconductor. Then the particle-hole and Majorana conditions can also be concisely expressed as

$$\gamma_E = \begin{cases} \gamma_{-E}^\dagger, & \text{PHS condiction} \\ \gamma_E^\dagger, & \text{Majorana condiction} \end{cases}$$

Trivially both conditions are satisfied at zero energy for $u_{j,0} = v_{j,0}^\dagger$.

It is not always possible to impose the Majorana conditions for the zero modes in superconductors. In a spin-singlet superconductor, an excitation has the structure

$$\gamma_\alpha^\dagger = \sum_j u_{j,\alpha} c_{j,\alpha}^\dagger + v_{j,-\alpha} c_{j,-\alpha}$$

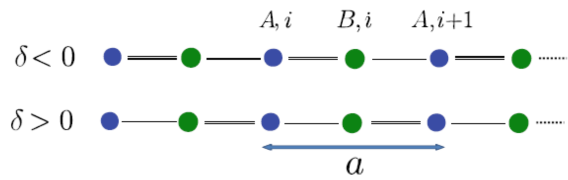
where α is a spin index $\uparrow/\downarrow$. Now j runs only over the site and orbital degrees of freedom. The Majorana condition reads $\gamma_\alpha^\dagger = \gamma_\alpha$, and the quasiparticle and the antiquasiparticle contain different electron and hole creation operators. Hence, no matter the value of the coherence factors $(u_{j,\alpha}, v_{j,\alpha})$, it is not possible to create a Majorana fermion. In conclusion, a spin-singlet superconductor does not allow naturally the formation of Majorana fermions.

Su-Schrieffer-Hegger model

In this part, we describe the topological phases for two important models in one dimension, namely, the Su-Schrieffer-Hegger (SSH) and Kitaev models. We start with the SSH model.

The SSH model is a simple one dimensional hopping model originally introduced by Su, Schrieffer and Heeger (SSH) to describe certain aspects of polyacetylene. Consider the following tight binding model

$$H = -\sum_{n=1}^{N} (t+\delta)\left[\left(c_{An}^\dagger c_{Bn} + h.c\right) + (t-\delta)\left(c_{An+1}^\dagger c_{Bn} + h.c\right)\right]$$



where $n_{in} = c_{in}^\dagger c_{in}$ is the particle number operator, $t + \delta$ is called the long hopping parameter, $t - \delta$ is the short hopping parameter, and (A, B) are the two sublattices. The transformation $\delta \to -\delta$ changes the phase of the system, because the long hopping parameters become the short one. In the figure, we illustrate the two phases one with $\delta < 0$ and the other with $\delta > 0$. Nevertheless, they have different topology for open boundary conditions, because they have different topological invariants.

We are going to obtain the Bloch Hamiltonian that gives the function $h(k)$. This is obtained by the Fourier transform. The Fourier transform of the annihilation operators for the A and B are

$$a_k = \frac{1}{\sqrt{N}} \sum_n \exp(-ikna)\, c_{An} \quad \text{and} \quad b_k = \frac{1}{\sqrt{N}} \sum_n \exp(-ikna)\, c_{Bn}$$

Furthermore, the orthogonality of exponential function reads

$$\sum_n \exp[-ina(k-q)] = N\delta_{kq}$$

Substitute the above three equations into H, we find the Bloch Hamiltonian of the SSH model, given by

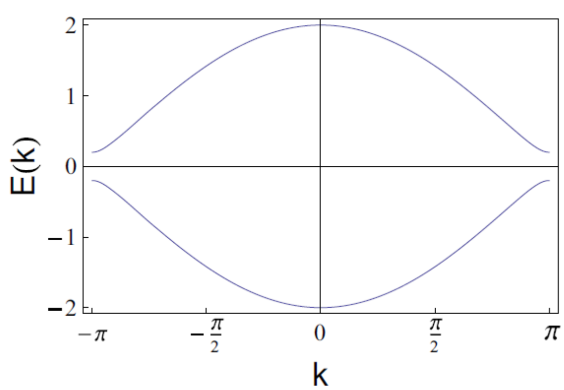
$$H = \sum_k \psi_k^\dagger \left(d_x \sigma_x + d_y \sigma_y\right) \psi_k$$

where $\psi_k^\dagger = (a_k \quad b_k)$ is a spinor field, σ_x and σ_y are the usual Pauli matrix, and

$$d_x = (t+\delta) + (t-\delta)\cos k$$

$$d_y = (t-\delta)\sin k$$

For the sake of simplicity, we have considered $a = 1$. The eigenvalues of the Bloch Hamiltonian are



$$E_\pm(k) = \pm\sqrt{d_x^2 + d_y^2} = \pm 2\sqrt{t^2\cos^2\left(\frac{k}{2}\right) + \delta^2\sin^2\left(\frac{k}{2}\right)}$$

In the figure above, we plot the energy eigenvalues. At the point $k = \pi$, the energy gap is 2δ. Therefore, the gap only closes if $\delta \to 0$. In this case, we break the adiabatic condition in the Hamiltonian, hence there exist a topological phase transition.

For the SSH model, the winding number is given by

$$v_{SSH} = -\frac{i}{2\pi}\int_{B.Z.} dk\hat{d}^{-1}(k)\partial_k \hat{d}k$$

where $\hat{d}k = d(k)/|d(k)|$ with $d(k) = d_x(k) + id_y(k)$. In general grounds, because the integral in v_{SSH} is over the first BZ $k \in [-\pi, \pi]$, the winding v_{SSH} can remove the hats

$$v_{SSH} = -\frac{i}{2\pi}\int_{B.Z.} dkd^{-1}(k)\partial_k dk$$

After some simplifications, we reach

$$v_{SSH} = \frac{1}{2}(1 - \text{sign}\delta)$$

Therefore, the winding number of the SSH model is

$$v_{SSH} = \begin{cases} 1, & \delta < 0 \\ 0, & \delta > 0 \end{cases}$$

The phase with nonzero winding number has zero-energy states. Indeed, it is easy to show that for $N = 4$, the Hamiltonian in reads

$$H = \mathcal{C}^\dagger \begin{pmatrix} 0 & -(t+\delta) & 0 & 0 \\ -(t+\delta) & 0 & -(t-\delta) & 0 \\ 0 & -(t-\delta) & 0 & -(t+\delta) \\ 0 & 0 & -(t+\delta) & 0 \end{pmatrix} \mathcal{C}$$

where $\mathcal{C}^\dagger = \begin{pmatrix} c_{A,1}^\dagger & c_{B,1}^\dagger & c_{A,2}^\dagger & c_{B,2}^\dagger \end{pmatrix}$ is the basis. The generalization for any N is straightforward. We have to calculate the eigenvalues of the above H. In Fig. 3 and 4, we plot the eigenvalues for each site n with $N = 100$, and $t = 1$. In the Fig. 3, we assume $\delta = -0.1$, thereby we have obtained that the SSH model has zero-energy states. In Fig. 4, we assume $\delta = 0.1$, then we obtained that the system has no zero-energy states.

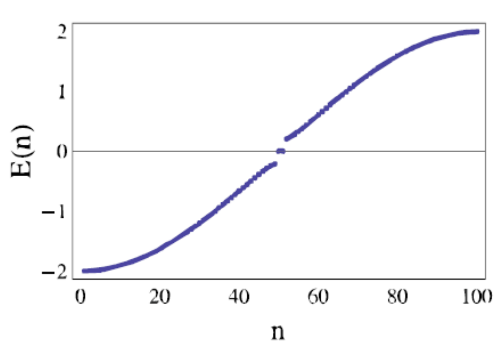


Fig. 3 The eigenvalues of the SSH model for $N = 100$, $t = 1.0$, and $\delta = -0.1$

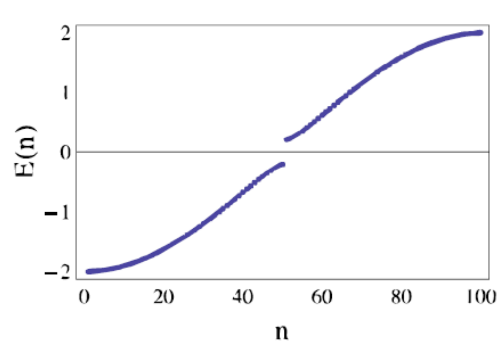


Fig. 4 The eigenvalues of the SSH model for $N = 100$, $t = 1.0$, and $\delta = +0.1$

From the particle-hole symmetry, we conclude that for each sate with energy E, there is other state with energy $-E$. Therefore, the zero-energy mode $E = 0$ must be double degenerate.

Next, let's start from the creation and annihilation operators $c^\dagger$ and c of a fermionic mode. These operators satisfy the anticommutation relation $c^\dagger c + cc^\dagger = 1$ and, furthermore, square to zero, $c^2 = 0$ and $(c^\dagger)^2 = 0$. They connect two states $|0\rangle$ and $|1\rangle$ which correspond to the 'vacuum' state with no particle and the 'excited' state with one particle, according to the following rules $c|0\rangle = 0$, $c^\dagger|0\rangle = |1\rangle$ and $c^\dagger|1\rangle = 0$.

When you have a pair of c and $c^\dagger$ operators, you can write them down in the following way

$$c^\dagger = \frac{1}{2}(\eta + i\gamma), \quad c = \frac{1}{2}(\eta - i\gamma)$$

The operators η, γ are known as Majorana operators. By inverting the transformation above, you can see that $\eta = \eta^\dagger$ and $\gamma = \gamma^\dagger$. Because of this property, we cannot think of a single Majorana mode as being 'empty' or 'filled', as we can do for a normal fermionic mode. This makes Majorana modes special.

You can also check that to maintain all the properties of c and $c^\dagger$, the operators η and γ must satisfy the following relations:

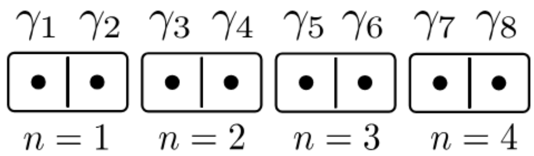
$$\eta\gamma + \gamma\eta = 0, \quad \eta^2 = 1, \quad \gamma^2 = 1$$

You can see that Majorana modes are similar to normal fermions in the sense that they have operators which all anticommute with each other. Using Majorana modes instead of normal fermionic modes is very similar to writing down two real numbers in place of a complex number. Indeed, every fermion operator can always be expressed in terms of a pair of Majorana operators. This also means that Majorana modes always come in even numbers.

The two Majorana operators η, γ still act on the same states $|0\rangle$ and $|1\rangle$. If these two states have an energy difference ϵ, this corresponds to a Hamiltonian $H = \epsilon c^\dagger c$. We can also express this Hamiltonian in terms of Majoranas as $H = \frac{1}{2}\epsilon(1 - i\eta\gamma)$.

Unpaired Majorana modes

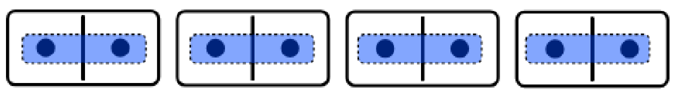
Let's see how creating isolated Majoranas can be done. Let us consider a chain of N sites, where each site can host a fermion with creation operator $c_n^\dagger$. Equivalently, each site hosts two Majorana modes γ_{2j-1} and γ_{2j}. This situation is illustrated below for N=4, where each site is represented by a domino tile.



What happens if we pair the Majoranas? This means that the energy cost for each fermion to be occupied is μ, and the Hamiltonian becomes

$$H = (i/2)\mu \sum_{j=1}^{N} \gamma_{2j-1}\gamma_{2j}$$

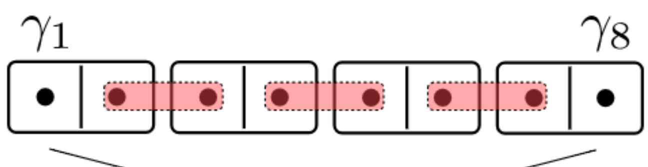
This is how the pairing looks:



no unpaired Majoranas

All the excitations in this system have an energy $\pm|\mu|/2$, and the chain has a gapped bulk and no zero energy edge states.

Of course this didn't help us to achieve our aim, so let's pair the Majoranas differently. We want only one Majorana to remain at an edge, so let's pair up the Majoranas from adjacent sites, leaving the first one and the last one without a neighboring partner:



unpaired Majorana modes

To every pair formed in this way, we assign an energy difference $2t$ between the empty and filled state, hence arriving at the Hamiltonian

$$H = it \sum_{j=1}^{N-1} \gamma_{2j}\gamma_{2j+1}$$

You can see that the two end Majorana modes γ_1 and γ_{2N} do not appear in H at all. Hence our chain has two zero-energy states, localized at its ends. All the states which are not at the ends of the chain have an energy of $\pm|t|$, independently on the length of the chain. Hence, we have a one-dimensional system with a gapped bulk and zero energy states at the edges.

The Kitaev chain model

Let us now try to write the Hamiltonian H, which we have so far written in terms of Majoranas, in terms of regular fermions by substituting $\gamma_{2j-1} = \left(c_j^\dagger + c_j\right)$ and $\gamma_{2j} = -i\left(c_j^\dagger - c_j\right)$. We find that both pairings sketched above are extreme limits of one tight-binding Hamiltonian for a one-dimensional superconducting wire:

$$H = -\sum_{j=1}^{N-1}\left[t\left(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j\right) - \frac{\Delta}{2}\left(c_j c_{j+1} + c_{j+1}^\dagger c_j^\dagger\right)\right] - \mu\sum_{j=1}^{N} n_j$$

where the Δ-term is due to the superconductor that breaks the Gauge symmetry $c_j \to c_j e^{i\phi}$, but preserves the discrete symmetry $c_j \to -c_j$. The t and μ terms are the usual hopping parameter between different sites and the onsite energy, respectively. $n_j = c_j^\dagger c_j$ is the particle number operator at the site j.

We apply the Fourier transform in the creation and annihilation operators, given by

$$c_j^\dagger = \frac{1}{\sqrt{N}}\sum_k \exp\left(-ikx_j\right)c_k^\dagger, \qquad k \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right], \quad x_j = ja$$

Using the above two equations, we find

$$H = \sum_k \epsilon_k c_k^\dagger c_k + \frac{\triangle}{2}\sum_k\left(e^{ika}\, c_{-k}\, c_k + e^{ika} c_k^\dagger c_{-k}^\dagger\right)$$

where $\epsilon_k = -2t\cos(ka) - \mu$.

Since the sum over the k is symmetric and $\epsilon_k = \epsilon_{-k}$, we have the identity

$$\sum_k \epsilon_k c_k^\dagger\, c_k = \frac{1}{2}\sum_k \epsilon_k\left(c_k^\dagger\, c_k + c_{-k}^\dagger\, c_{-k}\right) = \frac{1}{2}\sum_k \epsilon_k\left(c_k^\dagger\, c_k - c_{-k} c_{-k}^\dagger + 1\right)$$

Substitute the above equation into the Hamiltonian but neglecting the term $1/2\sum_k \epsilon_k$, which is just an overall constant, we obtain

$$H = \frac{1}{2}\sum_k \mathcal{C}_k^\dagger H_{kk}\mathcal{C}_k$$

where the basis is $\mathcal{C}_k^\dagger = \left(c_k^\dagger,\ c_{-k}\right)$, H_{kk} is the Bloch Hamiltonian of the Kitaev model, given by

$$H_{kk} = \vec{\sigma}\cdot\mathbf{d}(\mathbf{k}) = \begin{pmatrix} -\mu - 2t\cos(ka) & -2i\Delta\sin(ka) \\ 2i\Delta\sin(ka) & \mu + 2t\cos(ka) \end{pmatrix}$$

where $\vec{\sigma}$ are the Pauli matrix and $\mathbf{d}(\mathbf{k}) = (\Delta\cos(ka), \Delta\sin(ka), \epsilon_k)$. This is also known as Bogoliubov-de Gennes (BdG) Hamiltonian.

The eigenvalues of the Bloch Hamiltonian H_{kk} are (bulk energy dispersion)

$$E(k,\Delta) = \pm\sqrt{4|\Delta|^2\sin^2(ka) + (2t\cos(ka) + \mu)^2}$$

Therefore the bulk gap closes for $k = 0$ and $\mu = -2t$, or $k = \pi/a$ and $\mu = 2t$. This is natural: Since our chain does not have boundaries anymore, the energy spectrum does not contain the zero energy Majorana modes.

At first sight, the band structure looks quite similar on both sides of the bulk gap closings. Just from the above plot, it is not clear that the bulk gap closings separate two distinct phases of the model.

Study of the bulk transition with an effective Dirac model

Let's look at the gapless points more in detail. We focus on the gap closing at $\mu = -2t$, which happens at $k = 0$. Close to this point where the two bands touch, we can make a linear expansion of the Hamiltonian $H(k)$,

$$H(k) \cong m\tau_z + 2\Delta k\tau_y$$

With $m = -\mu - 2t$. We can see that $H(k)$ becomes a Dirac Hamiltonian. You can easily check that this Hamiltonian gives an energy spectrum $E(k) = \pm\sqrt{m^2 + 4\Delta^2 k^2}$, and by returning to the plot above you can indeed verify that this is a very good approximation of the exact band structure around $\mu = -2t$.

The "mass" m appearing in this Dirac Hamiltonian is a very important parameter to describe what is happening. Its magnitude is equal to the energy gap $|\mu + 2t|$ in the band structure close to the gap closing. Its sign reminds us of the two original phases with trivial and non-trivial topology:

- $m < 0$ for $\mu > -2t$, which corresponds to the topological phase, the one with Majorana modes in the open chain.
- $m > 0$ for $\mu < -2t$, which corresponds to the trivial phase, the one without Majorana modes in the open chain.

Previously, we had identified the point $\mu = -2t$ as a phase transition between two phases with or without zero energy edge modes. By looking at the bulk Hamiltonian, the same point $\mu = -2t$ appears as a point where the bulk gap closes and changes sign.

When $m = 0$, the Hamiltonian has two eigenstates with energy $E = \pm 2\Delta k$. These states are the eigenstates of τ_y, hence they are equal weight superpositions of electron and holes. They are in fact Majorana modes, that are left-moving on the branch $E = -2\Delta k$ and right-moving on $E = 2\Delta k$. Now they are free to propagate in the chain since there is no bulk gap anymore. In our simple model, the speed of these modes is given by $v = 2\Delta$.

Let's go back to the Kitaev model. Without the superconductor, we have $E(\pm\pi/a, 0) = \pm|2t + \mu| = \pm\big|2t - |\mu|\big|$ with $\mu < 0$. Therefore, if the system cross the point $2t = |\mu|$, the gap closes and topology changes. Nevertheless, contrary to the SSH model, the nontrivial phase of the

Kitaev model implies in the existence of Majorana fermions at the end of the chain. The Majorana operators η_j and γ_j at each site j are

$$c_j = \frac{1}{2}(\eta_j + i\gamma_j)$$

where (η_j, γ_j) are reals. Due to the anti-commutative properties $\{c_j^\dagger, c_k\} = \delta_{jk}$ and $\{c_j, c_k\} = 0$, we have

$$(\gamma_j, \eta_k) = 0, \quad (\eta_j, \eta_k) = 2\delta_{jk}, \quad (\gamma_j, \gamma_k) = 2\delta_{jk}$$

The main goal is to convert the Kitaev Hamiltonian in the tight-binding, using the equations in above two lines, from the electron operators to Majorana operators. This procedure may be done for any fermionic model.

The tight-binding becomes

$$H = \sum_{j=1}^{N-1} \frac{ti}{2}(\eta_{j+1}\gamma_j - \gamma_{j+1}\eta_j) - \frac{\Delta i}{4}(\eta_{j+1}\gamma_j + \gamma_{j+1}\eta_j) + \frac{\mu i}{2}\sum_{j=1}^{N} \gamma_j \eta_j$$

For the sake of simplicity, we shall consider $\mu = 0$ and $t = \Delta/2$ in the above Hamiltonian. Therefore

$$H = -\frac{\Delta i}{2}\sum_{j=1}^{N-1} \gamma_{j+1}\eta_j$$

Remarkably, the competition between the hopping parameter t and the coupling Δ has eliminated two boundary-Majorana operators. Majorana fermions are coupled only between neighboring sites. Then two unpaired Majorana fermions remain at the ends of the chain. They are completely localized at the extremity sites and have zero energy as they are decoupled from the Hamiltonian.

The topological phase was characterized by a $\mathbb{Z}_2$ topological invariant denoted by M as we discussed before. If the wire supports Majorana fermions, then $M = -1$, and, if the system is in a trivial gapped phase, then $M = 1$. When the bulk gap closes, M is undefined.

The Hamiltonian can be expanded in a basis of particle-hole Pauli matrices τ

$$\mathcal{H}_{BdG} = H_{kk} = h_y\tau_y + h_z\tau_z$$

with $h_y = 2\Delta\sin(ka)$ and $h_z = -\mu - 2t\cos(ka)$. Note that the system obeys the TRS, represented by the operator of complex conjugation K and the chiral symmetry. Also note that the unit vector Hamiltonian, $\hat{\mathrm{h}}$, is a mapping from the one dimensional torus $\mathbf{T}^1$ to the circle $\mathbf{S}^1$. Therefore the behavior of h can be characterized by a winding number w

$$w = -\frac{1}{2}\sum_{k\in\{0,\pi\}} \mathrm{sign}\big(h_z \partial_k h_y\big) = \frac{1}{2}[\mathrm{sign}(2t-\mu) + \mathrm{sign}(2t+\mu)]$$

where the sum was performed over the nodes of the dispersion ($k = 0$ and $k = \pi$). The winding number is either zero, for $|\mu| > 2|t|$, and there are no edge states inside the gap, or one, for $|\mu| < 2|t|$, and it is a Majorana bound state inside the gap.

This allows to relate the winding number to the M topological index:

$$M = \begin{cases} -1, & |\mu| < 2|t| \\ 1, & |\mu| > 2|t| \end{cases}$$

where $M = 1$ denotes that the trivial strong-pairing phase and $M = -1$, the weak pairing phase (the topological phase). When the bulk gap closes, M is undefined.

Note that because the system is described by a $\mathbb{Z}_2$ invariant, it could sustain multiple Majorana modes at a given edge. The fact that there are only two topological phases is entirely due to the fact that it involves only nearest-neighbor couplings.

A different evaluation of the topological invariant M is given by

$$M = (-1)^{\nu(\pi)-\nu(0)}$$

where $\nu(k)$ is the number of negative eigenvalues of H_{BdG} at the k point. Here [0, π] is half the BZ and then $\nu(\pi) - \nu(0)$ is the number (mod 2) of Fermi points in half-BZ. This definition relies on the existence of the PHS symmetry that ensures that the other half of the BZ has the same number of Fermi points.

Therefore the conditions to have Majorana fermions in the system are, up to now: having a spinless or spin-triplet superconductor, a bulk gap, and an odd number of Fermi points in half the BZ.

Pfaffian invariant

We have just seen that the gap closing in the Kitaev chain model is accompanied by a change of sign of M. This suggests to try to link the quantity M to a Pfaffian.

In fact, you can think of the full $\mathcal{H}_{BdG}$ as a very large matrix with particle-hole symmetry. It can be put in antisymmetric form and we can compute its Pfaffian. This Pfaffian may change only when an eigenvalue of H(k) passes through zero. Because of particle-hole symmetry, for every eigenvalue E(k) we have one at $-E(-k)$. So if $E(k)$ passes through zero, also its partner does. Furthermore, the spectrum has to be periodic in the Brillouin zone, which means that gap closings at finite momentum always come in pairs, and cannot change the Pfaffian. There are only two points which make exception: k=0 and k=π, which are mapped onto themselves by particle-hole symmetry. In fact, for these points we have:

$$\tau_x \mathcal{H}^*(0)\tau_x = -\mathcal{H}(0)$$

$$\tau_x \mathcal{H}^*(\pi)\tau_x = -\mathcal{H}(\pi)$$

So $\mathcal{H}(0)$ and $\mathcal{H}(\pi)$ can always be put individually in antisymmetric form, and we can always compute their Pfaffian. Also, note that these are precisely the points in momentum space where the gap closes: at k=0 for μ=−2t and at k=π for μ=2t. All things considered, we have a strong reason to focus exclusively on $\mathcal{H}(0)$ and $\mathcal{H}(\pi)$. Following the procedure that we learned in the last chapter, we can therefore put $\mathcal{H}(0)$ and $\mathcal{H}(\pi)$ in antisymmetric form,

$$\mathcal{H}(0) = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}\begin{pmatrix} -2t-\mu & 0 \\ 0 & 2t+\mu \end{pmatrix}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} = -i\begin{pmatrix} 0 & -2t-\mu \\ 2t+\mu & 0 \end{pmatrix}$$

$$\mathcal{H}(\pi) = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}\begin{pmatrix} 2t-\mu & 0 \\ 0 & -2t+\mu \end{pmatrix}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} = -i\begin{pmatrix} 0 & 2t-\mu \\ -2t+\mu & 0 \end{pmatrix}$$

We now easily obtain that

$$\mathrm{Pf}[i\mathcal{H}(0)] = -2t-\mu$$

$$\mathrm{Pf}[i\mathcal{H}(\pi)] = 2t-\mu$$

You see that the Pfaffian of $\mathcal{H}(0)$ changes sign at μ=−2t, and the Pfaffian of $\mathcal{H}(\pi)$ does so at μ=2t, in perfect agreement with the position of the gap closing in the band structure.

Individually, the two Pfaffians account for one of the two bulk gap closings which can occur in the model. To obtain a single bulk invariant M we can simply multiply the two! Hence we arrive at the following expression:

$$M(\mathcal{H}) = \mathrm{sign}(\mathrm{Pf}[i\mathcal{H}(0)]\mathrm{Pf}[i\mathcal{H}(\pi)])$$

A value $M = -1$ means that the bulk is in a topological phase, such that if the wire was cut at a point, two unpaired Majorana modes would appear at the ends of it. On the other hand, a value $M = +1$ means that the bulk is in the trivial phase. The topological invariant M cannot change under continuous deformations of the Hamiltonian unless the gap closes.

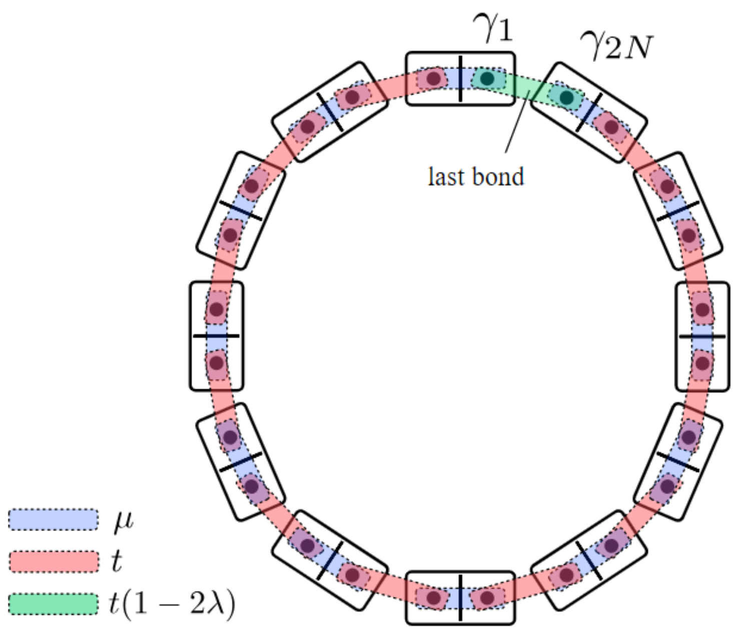
Connecting the bulk invariant and the edge modes

We will give a more concrete physical meaning to the value of M. We have already connected the Pfaffian of a BdG Hamiltonian to a physical quantity: The ground state fermion parity of the system. Our one-dimensional invariant involves the product of two Pfaffians, $\mathrm{Pf}[i\mathcal{H}(0)]$ and $\mathrm{Pf}[i\mathcal{H}(\pi)]$. By taking their product we are somehow comparing the fermion parity of the two states of the chain with k=0 and k=π, and we have that $M = -1$ if and only if the two parities are different. This means that if we continuously deform $\mathcal{H}(0)$ into $\mathcal{H}(\pi)$ in some way without breaking the particle-hole symmetry, we must encounter a zero-energy level crossing in the energy spectrum, what we called a fermion parity switch.

In practice, this can be done in the following way. Let's imagine that we change the boundary conditions of a Kitaev ring with N sites from periodic to antiperiodic boundary conditions, that is from $\langle k|n=0\rangle = \langle k|n=N\rangle$ to $\langle k|n=0\rangle = -\langle k|n=N\rangle$. This means that the allowed values of momentum shift from $2\pi k/N$ to $2\pi k/N + \pi/N$.

Let's now ask what is the difference in ground state fermion parity of the two chains. The value k=0 is always present in the chain with periodic boundary conditions, while k=π is in the first set if N is even and in the second set if N is odd. This means that in either case, the difference in the ground state fermion parities between the chains with periodic and antiperiodic boundary conditions is equal to M.

To verify this statement, we will now physically change the boundary condition in real space. For simplicity, we will do so for a Kitaev ring with Δ=t. You will remember that, in the Majorana basis, this corresponds to the limit where neighboring Majoranas from different sites are coupled by hopping of strength t. To go from periodic to antiperiodic boundary condition, we can change the hopping on the last bond of the ring (the one connecting sites n=N−1 and n=0) from t to −t. This can easily be done continuously and without breaking particle-hole symmetry, for instance by setting the last hopping to be equal to t(1−2λ) and varying λ in the interval [0,1], as shown in this picture:



You can see that for μ<2t, the energy spectrum shows a zero-energy level crossing at λ=1/2. The fermion parity of the system is therefore different at λ=0 and λ=1. When λ=1/2 the hopping on the last bond is equal to zero. We have introduced a "cut" to the system, such that our closed Kitaev ring is effectively transformed to an open Kitaev chain. Because we are in the topological phase, this open Kitaev chain has two zero-energy unpaired Majorana modes!

On the other hand, when μ>2t no zero-energy level crossing is present. The ground state fermion parity is the same at λ=0 and λ=1. In this case, when we cut the system at λ=1/2, we find no unpaired Majorana modes, consistent with our knowledge of the behavior of the open chain in the trivial phase.

We have therefore learned the essence of the bulk-boundary correspondence: A non-trivial value $M=-1$ of the bulk invariant for the closed chain implies the existence of unpaired Majorana modes for the open chain. Also, we have been able to connect the value of the bulk invariant to a measurable quantity, in this case the ground state fermion parity of the closed chain.